Bloch electron in a magnetic field and the Ising model

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The spectral determinant $\det(H-\varepsilon I)$ of the Azbel-Hofstadter Hamiltonian H is related to Onsager's partition function of the 2D Ising model for any value of magnetic flux $\Phi = 2\pi P/Q$ through an elementary cell, where P and Q are coprime integers. The band edges of H correspond to the critical temperature of the Ising model; the spectral determinant at these (and other points defined in a certain similar way) is independent of P. A connection of the mean of Lyapunov exponents to the asymptotic (large Q) bandwidth is indicated.

Although the problems of an electron in a constant magnetic field and that of an electron on a periodic lattice were solved in the early days of quantum mechanics, the case where a magnetic field and a lattice are present simultaneously still defies adequate understanding. The simplest model for this case is commonly referred to as the Hofstadter or Azbel-Hofstadter model [1,2]. The corresponding Hamiltonian describes an electron on a two-dimensional (2D) $N \times N$ square lattice with nearest-neighbour hopping subject to a perpendicular uniform magnetic field:

$$\begin{aligned}(H\psi)_{n_x,n_y} &= \psi_{n_x-1,n_y} + \psi_{n_x+1,n_y} + \\ &\lambda e^{-in_x\Phi}\psi_{n_x,n_y-1} + \lambda e^{in_x\Phi}\psi_{n_x,n_y+1}, \\ &n_x, n_y = 0, 1, \ldots, N-1,\end{aligned} \tag{1}$$

where $\Phi = 2\pi P/Q$ is the flux through an elementary cell (measured in units of the elementary flux), P and Q are coprime (that is they do not have a common divisor other than 1) positive integers, $\lambda = t_1/t_2 \geq 0$ is a ratio of hopping amplitudes in the x and y directions. We impose the periodic boundary conditions ($\psi_{N,n_y} = \psi_{0,n_y}$, $\psi_{-1,n_y} = \psi_{N-1,n_y}$, similarly for n_y). Usually, the Hamiltonian (1) is defined on an infinite lattice at the outset; in the present paper, however, we shall deal first with a finite N and take the limit $N \to \infty$ later on.

This Hamiltonian and the related one-dimensional operator were studied in many works (see [3–5] for reviews). Nevertheless, the quantitative description of the spectrum remains to a large extent an open problem. Hamiltonian (1) is related to that of a quantum particle on a line in the presence of two periodic potentials. It is the effect of incommensurability of the periods (when $\Phi/2\pi$ is irrational or, in other words, $P, Q \to \infty$) leading to the fractal structure of the spectrum that makes the problem both difficult and interesting. Its solution would be an essential contribution to the theory of fractals, would be important for studies of localization-delocalization phenomena, the quantum Hall effect, as well as purely for number theory and functional analysis.

It was noticed by Wiegmann and Zabrodin [6] that the model is related to integrable systems and the algebra $U_q(sl_2)$. This was generalized in [7]. In the present paper, we find a different type of relation to integrable systems. We shall see that the spectral determinant $\det(H-\varepsilon I)$ for any $\Phi = 2\pi P/Q$ is simply mapped onto Onsager's partition function of the 2D Ising model (formulas (8)–(10)). This relation is, in a sense, complementary to the one established in [6,7]: we shall explain this later in the text.

In the present paper, we remove part of the mystery about the Thouless conjecture on the total bandwidth. It is well known that the spectrum of H for an infinite lattice (on $l_2(Z)$) consists of Q intervals (bands). When $Q \to \infty$, the total width W of the bands for $\lambda \neq 1$ is known [8] to approach $4|1-\lambda|$ exponentially fast in Q; for $\lambda = 1$, it is of order $1/Q$ [9]. Thouless formulated a conjecture [10,11] that for $\lambda = 1$ the total width $W \sim 32G/\pi Q$ as $Q \to \infty$, where $G = 1 - 1/3^2 + 1/5^2 - 1/7^2 \ldots$ is Catalan's constant. (Notation $A \sim B$ means, henceforth, that A/B tends to 1 in the limit.) This result was derived only for $P = 1$, $P = 2$ so far [11–14] but is supposed to hold in the general case (even when P/Q tends to *any* nonzero limit) for which it is supported by extensive numerical data; thus, the bandwidth is supposed to have an interesting universality property with respect to Φ. We shall generalize this conjecture and recast it into a simpler type of statement (expression (13)) by relating the quantity $\gamma(\varepsilon) = \lim_{N\to\infty}(1/N^2)\ln|\det(H-\varepsilon I)|$ (which is interpreted as a mean of Lyapunov exponents) to the bandwidth. In particular, for any band edge ε_{e_i}, *any* coprime P, Q, and $\lambda = 1$, we get an exact result: $\gamma(\varepsilon_{e_i}) = 4G/\pi Q$. This differs from the supposed asymptotic formula for the total bandwidth only by the factor 8.

First, let us use the translational symmetry of H in the x and y directions. Substitute $\psi_{n_x,n_y} = e^{ik_y n_y}\mu_{n_x}$, $k_y = 2\pi k/N$, $k = 0, 1, \ldots, N-1$ into (1) to get $H = \oplus_{k=0}^{N-1} H_k$, the eigenvalue equation for H_k being

$$(H_k\mu)_n =$$
$$\mu_{n-1} + \mu_{n+1} + 2\lambda \cos\left(\frac{2\pi P}{Q}n + \frac{2\pi k}{N}\right)\mu_n = \varepsilon\mu_n, \quad (2)$$
$$n = n_x = 0, 1, \ldots, N-1.$$

When n is allowed to range from $-\infty$ to ∞, the corresponding H_k on $l_2(Z)$ is called the almost Mathieu operator.

Let us assume that N is divisible by Q and substitute $\mu_{j+Ql} = e^{i\omega l}\xi_j$, $j = 0, 1, \ldots, Q-1$, $\omega = \frac{2\pi m}{N/Q}$, $m = 0, 1, \ldots, N/Q-1$ into (2). We get $H_k = \oplus_{m=0}^{N/Q-1} H_{km}$,

$$(H_{km}\xi)_j = \xi_{j-1} + \xi_{j+1} + 2\lambda\cos\left(\frac{2\pi P}{Q}j + \frac{2\pi k}{N}\right)\xi_j$$
$$j = 0, 1, \ldots, Q-1; \qquad \xi_Q = e^{i\omega}\xi_0, \qquad \xi_{-1} = e^{-i\omega}\xi_{Q-1}. \quad (3)$$

The Chambers formula [15] gives the dependence of the spectral determinant (characteristic polynomial) of H_{km} on k and m, namely:

$$\det(H_{km} - \varepsilon I_{Q\times Q}) = (-1)^Q\left(\sigma(\varepsilon) - 2\lambda^Q\cos\frac{2\pi k}{N/Q} - 2\cos\frac{2\pi m}{N/Q}\right), \quad (4)$$

where $\sigma(\varepsilon)$ is a polynomial of degree Q which depends on λ and Φ, but not on k and m. It is easy to verify (4) by considering the matrix given by (3) and the one obtained after the substitution $\xi_j = \sum_{l=0}^{Q-1}\exp 2\pi i(jlP/Q + jm/N + lk/N)\xi'_l$. It is the expression (4) which implies that the spectrum of H in the limit $N \to \infty$ consists exactly of Q bands: the image of the interval $[-2(1+\lambda^Q), 2(1+\lambda^Q)]$ under the inverse of the transform $\sigma = \sigma(\varepsilon)$ (see Fig. 1).

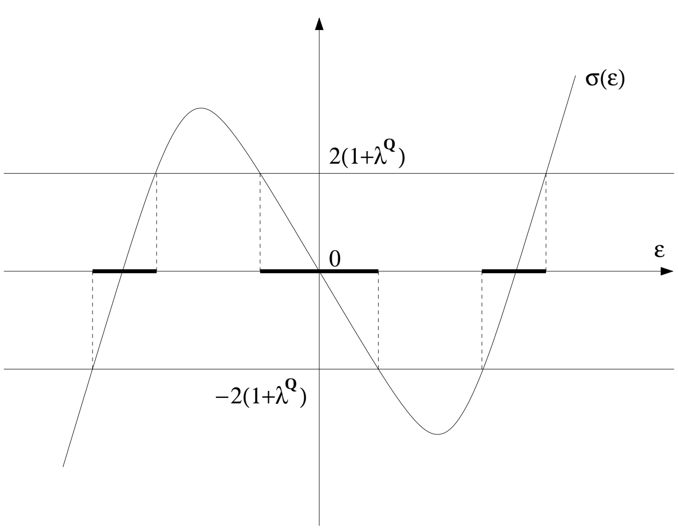

FIG. 1. The polynomial $\sigma(\varepsilon)$ is sketched for $Q = 3$. The bands of the spectrum are shown by thick lines.

Thus,

$$\det(H - \varepsilon I) = \prod_{k=0}^{N-1}\prod_{m=0}^{N/Q-1}\det(H_{km} - \varepsilon I_{Q\times Q}) = (-1)^{N^2}\prod_{k,m=0}^{N/Q-1}\left(\sigma(\varepsilon) - 2\lambda^Q\cos\frac{2\pi k}{N/Q} - 2\cos\frac{2\pi m}{N/Q}\right)^Q. \quad (5)$$

In the limit of infinite lattice ($N \to \infty$), let us replace $2\pi k/N$ in (2) by a continuous parameter θ, denote H_k by H_θ, and consider the mean $\gamma(\varepsilon)$ of Lyapunov exponents over all real θ. By virtue of the 3-term recursion (2), any μ_n is obtained from initial conditions μ_0, μ_1. The Lyapunov exponent $\gamma_\theta(\varepsilon)$ corresponding to H_θ describes the exponential rate of growth (or decay) of a solution to the equation $(H_\theta\mu)_n = \varepsilon\mu_n$, $n = 0, 1, \ldots$. More precisely,

$$\gamma_\theta(\varepsilon) = \lim_{n\to\infty} n^{-1}\max_{\mu_0,\mu_1;\ \mu_0^2+\mu_1^2=1}\ln(\mu_n^2 + \mu_{n+1}^2)^{1/2}. \quad (6)$$

Note that the difference between H_θ defined in the space of square-summable sequences with indices $n = 0, 1, \ldots$ and the almost Mathieu operator corresponding to $n = \ldots, -1, 0, 1, \ldots$ is that the spectrum of the latter is doubly degenerate. However, the normalized to unity density of states $\rho_\theta(x)$ is the same in both cases. According to the Thouless formula [16], $\gamma_\theta(\varepsilon) = \int \ln|\varepsilon - x|\rho_\theta(x)dx$. Using this formula and (5), we get for the mean of $\gamma_\theta(\varepsilon)$ over θ (to ensure that the determinant is nonzero we assume that ε has an imaginary part; after taking the limit $N \to \infty$ we can let $\Im\varepsilon \to 0$):

$$\gamma(\varepsilon) = \lim_{N\to\infty}\frac{1}{N^2}\ln|\det(H - \varepsilon I)| = \frac{1}{\pi^2 Q}\int_0^\pi\int_0^\pi \ln|\sigma(\varepsilon) - 2\lambda^Q\cos x - 2\cos y|dxdy. \quad (7)$$

On the other hand, Onsager's partition function Z for the 2D Ising model on a square $N \times N$ lattice satisfies [17]:

$$\lim_{N\to\infty}\frac{1}{N^2}\ln Z - \frac{1}{2}\ln(2\sinh a') = \frac{1}{2\pi^2}\int_0^\pi\int_0^\pi \ln\left|2\frac{\cosh a\cosh a'}{\sinh a'} - 2\frac{\sinh a}{\sinh a'}\cos x - 2\cos y\right|dxdy. \quad (8)$$

Here $a = 2J/T$, $a' = 2J'/T$, where T is the temperature; J, J', interaction constants in x and y direction. We now set $\sinh a/\sinh a' = \lambda^Q$ (hence $a' = \operatorname{arcsinh}(\lambda^{-Q}\sinh a)$);

$$\sigma(\varepsilon) = 2\frac{\cosh a\cosh a'}{\sinh a'} = 2\lambda^Q\coth a\sqrt{1 + \lambda^{-2Q}\sinh^2 a}; \quad (9)$$

to obtain the equivalence (as $N \to \infty$) for any ε and coprime P and Q:

$$|\det t_2(H - \varepsilon I)| \sim Z^{2/Q}, \tag{10}$$

where $t_2^Q = 2\sinh a'$.

A simple analysis of (9) shows that for any real T, $|\sigma(\varepsilon)| \geq 2(1+\lambda^Q)$. The minimum of $|\sigma(\varepsilon)|$ as a function of T, $|\sigma(\varepsilon)| = 2(1+\lambda^Q)$, corresponds to the critical temperature T_c of the Ising model (at T_c the argument of the logarithm in (7) and (8) vanishes at an integration limit). On the other hand, the energies ε_{e_i} at which $|\sigma(\varepsilon_{e_i})| = 2(1+\lambda^Q)$ are the band edges of $\lim_{N\to\infty} H$.

It is well known [18] that Z at T_c equals the square of the partition function Z_D of dimers on the lattice if $r_1 = \sqrt{2\sinh a}$ and $r_2 = \sqrt{2\sinh a'}$ are interpreted as activities of dimers in x and y directions. Let us identify $r_1^2 = t_1^Q$ and $r_2^2 = t_2^Q$ (recall that t_1 and t_2 are hopping amplitudes in x and y directions, and $\lambda = t_1/t_2$). One result of Lieb and Loss [19] says that $\det \widetilde{H} \sim Z_D^2$ as $N \to \infty$ for the flux $\Phi = \pi$, that is for $P = 1$, $Q = 2$. Here $\widetilde{H} = t_2 H$ — a more symmetric form of the Azbel-Hofstadter Hamiltonian. Since it is known that $\varepsilon = 0$ is a band edge for Q even, we have from (10) $\det \widetilde{H} \sim Z_D^{4/Q}$, which is a generalization of the mentioned result to any coprime P odd, Q even.

In the works [6,7] the Bethe ansatz equations are formulated for the zeros of the characteristic polynomial of H_{km}, in other words, for the roots of the equation $\sigma(\varepsilon) = \text{const}$. Thus [6,7] are to do with the "internal" structure of $\sigma(\varepsilon)$, whereas in our formalism $\sigma(\varepsilon)$ enters as an "indivisible" object and our results come from what appears (at least at first sight) "external" to $\sigma(\varepsilon)$ structure of the problem: the translational symmetry and the Chambers formula.

Henceforth, we only consider the limit of infinite N.

Let us simplify expression (7) (note an important fact that γ depends on ε and P only through $\sigma(\varepsilon)$!). Because of the obvious equality $\gamma(\sigma, \lambda) = \ln\lambda + \gamma(\sigma/\lambda^Q, 1/\lambda)$, it is sufficient to consider only the case $0 \leq \lambda \leq 1$. In this case, taking the integral over y in (7) we get:

$$\gamma(\sigma) = \begin{cases} \frac{1}{\pi Q}\int_0^{\pi} \operatorname{arccosh}(|\sigma|/2 + \lambda^Q \cos x)dx, \\ \qquad |\sigma| \geq 2(1+\lambda^Q); \\ \frac{1}{\pi Q}\int_0^{\arccos\{(2-|\sigma|)/2\lambda^Q\}} \operatorname{arccosh}(|\sigma|/2 + \lambda^Q \cos x)dx, \\ \qquad 2(1+\lambda^Q) > |\sigma| > 2(1-\lambda^Q); \\ 0, \qquad |\sigma| \leq 2(1-\lambda^Q). \end{cases} \tag{11}$$

The fact that $\gamma(\varepsilon)$ is zero on the image of the interval $\sigma \in [-2(1-\lambda^Q), 2(1-\lambda^Q)]$ is in agreement with the general argument: this image is an intersection of the intervals of the spectra of the operators H_θ. The generalized eigenfunction of any H_θ is just a Bloch wave on a periodic lattice with Q atoms in an elementary cell. Therefore, the Lyapunov exponents $\gamma_\theta(\varepsilon)$ are zero on this set. By definition, $\gamma(\varepsilon)$ is a mean of these exponents.

Let us remark that rather than considering $\det(H - \varepsilon I)$, it is possible to derive equations (11) making use of some known properties (see, e.g., [20]) of the monodromy operator.

Now we can note that in the limit $Q \to \infty$, σ fixed, $\gamma(\sigma)$ tends to the following Lyapunov exponent *on the spectrum* of H: $\gamma(\varepsilon) \to 0$ if $\lambda \leq 1$, $\gamma(\varepsilon) \to \ln\lambda$ if $\lambda > 1$, in accordance with a statement of Aubry and André [21]. (Naturally, we obtain the same asymptotic result for any individual $\gamma_\theta(\varepsilon)$.)

For T_c ($|\sigma| = 2(1+\lambda^Q)$), let us represent (11) in another form by reducing the integral to $\int_0^{\pi/2} \operatorname{arcsinh}(\lambda^{Q/2}\cos x)dx$ and then using differentiation w.r.t. the parameter. We get for any $\lambda > 0$:

$$\begin{aligned} \gamma(\varepsilon_{e_i}) &= \frac{4}{\pi Q}\int_0^{\lambda^{Q/2}} \frac{\arctan x}{x}dx = \\ &\ln\lambda + \frac{4}{\pi Q}\int_0^{\lambda^{-Q/2}} \frac{\arctan x}{x}dx. \end{aligned} \tag{12}$$

In what follows, we always consider (the most interesting from the point of view of bandwidth) case $\lambda = 1$. It is not, however, difficult to generalize the argument below to the case of any λ. For $\lambda = 1$, the expression (12) reads: $\gamma(\varepsilon_{e_i}) = 4G/\pi Q$. In these terms, the Thouless conjecture says that the total bandwidth behaves as $8\gamma(\varepsilon_{e_i})$ asymptotically for large Q. The following more general fact appears to hold and is supported by numerics.

Let $W(x)$ be the total length of the image of $[0, x]$ under the inverse of the transform $\sigma = \sigma(\varepsilon)$ (recall that the whole spectrum is the image of $[-4, 4]$, i.e., the total bandwidth is $W = W(-4) + W(4)$). Then for any coprime P and Q (including P changing with Q such that P/Q is not small) as $Q \to \infty$:

$$W(\sigma) \sim 4\gamma(\sigma) = \frac{2}{\pi Q}\int_0^{|\sigma|} K(x/4)dx, \qquad \sigma \in [-4, 4]. \tag{13}$$

The last equation is just another form of (11) for $\lambda = 1$; $K(k) = \int_0^{\pi/2}(1 - k^2\sin^2 x)^{-1/2}dx$ is the complete elliptic integral of the first kind; the "$\sim$" relation is our conjecture.

It is easy to derive (13) in the case $P = 1$, where we can use the known from semiclassics [13] asymptotic expression for $\sigma(\varepsilon)$. In this case, the main asymptotic contribution to $W(\sigma)$ comes from the bands in a small neighbourhood of $\varepsilon = 0$. These bands have width of order $1/Q \ln Q$, while the others are exponentially narrow. For $|\varepsilon| \ll 1$, $P = 1$, and $Q \to \infty$,

$$\sigma(\varepsilon) \sim 4\cosh(\varepsilon Q/4)\cos\left(\frac{\varepsilon Q}{2\pi}\ln\frac{4Q}{\pi} - 2\arg\Gamma\left(\frac{1}{2}+i\frac{\varepsilon Q}{4\pi}\right) - \frac{\pi Q}{2}\right). \tag{14}$$

Hence, the asymptotic contribution of an individual band to $W(\sigma)$ is

$$\frac{2\pi}{Q\ln Q}\arcsin\frac{|\sigma|/4}{\cosh(\varepsilon Q/4)}, \tag{15}$$

and the number of such bands in an interval $dt = d(\varepsilon Q/4)$ is $\frac{2}{\pi}\ln Q\frac{dt}{\pi}$. Therefore, the sum of all contributions

$$W(\sigma) \sim \frac{8}{\pi Q}\int_0^\infty \arcsin\frac{|\sigma|/4}{\cosh t}dt = \frac{2}{\pi Q}\int_0^{|\sigma|} K(x/4)dx = 4\gamma(\sigma), \tag{16}$$

which completes the derivation of (13) for $P=1$.

If we could show that for a general P, $W(\sigma) \sim c\gamma(\sigma)$, where c is independent of σ, then the value of c could be found using a result of Last and Wilkinson [22] that for any coprime P and Q, $\sum_{i=1}^{Q}|\sigma'(\varepsilon_i)|^{-1} = Q^{-1}$, where $\sigma(\varepsilon_i) = 0$, $i = 1,\ldots,Q$. This can be written as $|W'_\sigma(0)| = 1/Q$ (right or left derivative) because, obviously, $|W'_\sigma(\sigma)| = \sum_{i=1}^{Q}|\sigma'(\varepsilon_i)|^{-1}$, where $\sigma(\varepsilon_i) = \sigma$, $i = 1,\ldots,Q$. On the other hand, since $K(0) = \pi/2$, we have $|\gamma'_\sigma(0)| = 1/4Q$, which implies that $c = 4$.

Putting our results and conjectures together, we can roughly say that the logarithm of Onsager's partition function, the mean of the Lyapunov exponents, and the asymptotic bandwidth are basically the same object which is universal in that for a fixed value of σ, it does not depend on P.

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